BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(END SEMESTER EXAMINATION)

CLASS: M. Pharm **SEMESTER: IInd**
BRANCH: PHARMACY **SESSION: SP2023**

SUBJECT: MPC203T COMPUTER AIDED DRUG DESIGN

TIME: 3.00 Hours **FULL MARK: 75**

INSTRUCTIONS:

1. The missing data, if any, may be assumed suitably.
2. Before attempting the question paper, be sure that you have got the correct question paper.
3. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.

Q.1(a)	"Molecular modeling before the computer age was done by the CPK models". Explain this sentence in the context of historical times of molecular modeling and drug discovery.	[7]
Q.1(b)	Elaborate the terms:(1)Quantum Mechanics (ii) Molecular Mechanics (iiiSystematic Search	[8]
Q.2(a)	Elaborate the QSAR equation and elaborate on the descriptors commonly used for QSAR equation	[7]
Q.2(b)	Detail out the Craig Plot with the diagram	[8]
Q.3(a)	Explain the preparation of a molecule for 3 D QSAR studies step by step	[7]
Q.3(b)	Define the following(i)Bioactive Conformation (ii) CoMFA and ComSIA (iii)Es (iv) Training and test set	[8]
Q.4(a)	Define the following: (i) Tabu Search (ii) Monte Carlo Search (iii)Distance Geometry Search	[7]
Q.4(b)	How do you explain Topliss tree for aromatics and aliphatics in relation to design of better molecules with activity	[8]
Q.5(a)	Discuss the docking protocol of a ligand in the active site of protein in detail.	[7]
Q.5(b)	Define (i) Active Site (ii) Scoring (ii) Manual docking (iv) Calculation of sigma	[8]
Q.6(a)	Discuss in detail the ADME tools and their relevance in drug design	[7]
Q.6(b)	Elaborate the method of homology modelling with brief discussion in each step	[8]
Q.7(a)	Explain (i) Energy minimization (ii) Resonance and Inductive effect (iii) Hydrogen bond intra	[7]
Q.7(b)	Write notes on (i) Hansch equation (ii) Advantages of 3D QSAR over 2D QSAR	[8]

:::::26/04/2023 E:::::